Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Origin of High Electronic Quality in Solar Cell Absorber $CH_3NH_3PbI_3$ WANJIAN YIN, Soochow University, TINGTING SHI, University of Toledo, SUHUA WEI, Beijing Computational Science Research Center, YANFA YAN, University of Toledo — Thin-film solar cells based on $CH_3NH_3PbI_3$ halide perovskites have recently shown remarkable performance. First-principle calculations and molecular dynamic simulations show that the structure of pristine $CH_3NH_3PbI_3$ is much more disordered than the inorganic archetypal thin-film semiconductor CdTe. However, the structural disorders from thermal fluctuation, point defects and grain boundaries introduce rare deep defect states within the bandgaps; therefore, the material has high electronic quality. We have further shown that this unusually high electronic quality is attributed to the unique electronic structures of halide perovskite: the strong coupling between cation lone-pair Pb s orbitals and anion p orbitals and the large atomic size of constitute cation atoms. We further found that although $CH_3NH_3PbI_3$ GBs do not introduce a deep gap state, the defect level close to the VBM can still act as a shallow hole trap state. Cl and O can spontaneously segregate into GBs and passivate those defect levels and deactivate the trap state.

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Date submitted: 07 Nov 2015 Electronic form version 1.4